HAÜY-BRAVAIS LATTICE AND OTHER CRYSTALLOGRAPHIC DATA FOR SODIUM MOLYBDO-TELLURATE*

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PART I. METHOD OF DETERMINING THE AXIAL ELEMENTS

INTRODUCTORY

The object of this section is to show the method used to choose the set of axial elements which is in best possible agreement with the law of Bravais.

The ideal set of axial elements should not only lead to simple indices for the known forms, for a number of different sets will fulfill this condition, but, as has been emphasized by Friedel[1] it should also give as much information as possible on the existing forms:

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[1] Leçons de Cristallographie professées à la Faculté des Sciences de Strasbourg, Georges Friedel, *Paris*, Berger-Levrault Ed., **1926,** p. 127.

it should enable the reader to infer the list of forms present on the crystals and the order of importance of these forms, from a mere inspection of the given axial elements.

That such an ideal set of axial elements does not exist, strictly speaking, is well known. The importance of a face is defined by its *frequency* of occurrence and its more or less perfect *development*. In terms of rate of growth, *slow faces* are the most important as they occur most frequently and usually are dominant faces. The forms of a crystalline species do not only depend on the space-lattice, but also on certain *disturbing factors*, such as on the length of time and other conditions of crystallization, presence of foreign ions in the solution, symmetry of the motif, etc. There is, nevertheless, a certain lattice, called the *Bravais lattice*[2] by G. Friedel, which approaches the ideal and will account for the observed facts better than any other. *Only in this Bravais lattice* is the importance of a face an increasing function of its reticular density. Moreover, the importance of a face does *not* usually increase with the reticular density in any other arbitrary lattice, however simple the symbols of the existing forms may be in that lattice.

It is chiefly because this fact has been overlooked that the parameters of crystalline species listed to date in standard reference books form such an incoherent chaos. The best remedy available to-day for all these inconsistencies is to adopt axial elements which express the Law of Bravais.

The determination of the axial elements will be explained here in detail for the sake of the *method* itself. The *results* will be summarized in Part II.

MEASUREMENTS

The crystals belong to the pinacoidal class of the triclinic system. A total of fourteen forms were observed. Of these, ten were very good and four imperfect. The four imperfect forms being very rare, the existence of the center of symmetry cannot be questioned.

We observed the frequency of occurrence and the development of the forms on a number of crystals (over 20). We listed the forms in their order of decreasing importance, numbering them from 1 to

[2] We propose to call it *Haüy-Bravais lattice* instead, as it will be remembered that the term *Bravais lattices* has been used in English with a different meaning: the fourteen space-lattices that may be obtained by adding translations to the usual symmetry-operations (provided all these translations are greater than one-half the distance between the points of one of the seven primary lattices).

14. In the substance here studied, certain forms look equally important; we group them together, in parentheses, in the following manner:

$$(1, 2), (3, 4), (5, 6), (7, 8), 9, 10, 11, (12, 13, 14).$$

Besides the *five fundamental angles* necessary for our calculations, we measured several additional angles (eleven) against which the computed values were checked. The list of measured angles will be found in Table 1 (4th column). The faces are designated by their numbers in the 1st column; conventionally, 1′ will represent the face parallel to **1**, etc. An idea of the value of the series of measurements may be had from the 2nd and 3rd columns, giving respectively the number of measurements for each angle and the *probable error*. The value given under the heading "Measured" is in each case the *most probable value, i.e.* giving the *least mean quadratic error*.

The measurements were made with the non-modified type of a Wollaston reflection goniometer.
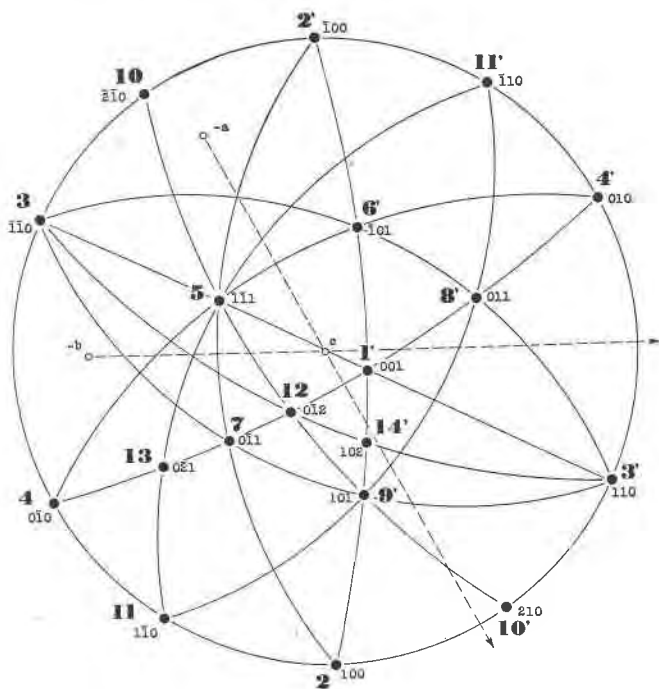

FIG. 1. Projection (I).

CALCULATION OF THE 1ST SET OF AXIAL ELEMENTS

A projection of the crystal is made by using a Wulff stereographic net (Fig. 1). A preliminary set of axial elements is determined by assigning simple Miller symbols to the most common and best developed faces: $1'(001)$, $2(100)$, $4'(010)$, $3'(110)$, and $6'(\bar{1}01)$. In this calculation, we use as fundamental data five interfacial angles chosen from those giving the best measurements.

TABLE 1

COMPARISON BETWEEN MEASURED AND COMPUTED ANGLES

Angle: (face numbers)	Number of readings	Probable error	Measured	Computed	Angle: (face symbols)	
					Lévy	Miller
$2 \wedge 4$	23	8.9′	62°56′	—	$g^1 \cdot e^1$	$010 \wedge 01\bar{1}$
$1 \wedge 4$	17	8.2′	79°58′	—	$h^1 \cdot e^1$	$\bar{1}00 \wedge 01\bar{1}$
$2' \wedge 3$	12	8.2′	63°40′	—	$g^1 \cdot p$	$0\bar{1}0 \wedge 00\bar{1}$
$1' \wedge 2$	18	9.9′	82°42′	—	$h^1 \cdot g^1$	$100 \wedge 010$
$1 \wedge 6$	13	12.1′	49°17′	—	$h^1 \cdot m$	$\bar{1}00 \wedge \bar{1}10$
$2 \wedge 6$	13	9.1′	47°52′	48° 1′	$g^1 \cdot m$	$010 \wedge \bar{1}10$
$1 \wedge 3$	11	9.6′	73° 1′	73° 9′	$h^1 \cdot p$	$\bar{1}00 \wedge 00\bar{1}$
$1' \wedge 5$	10	13.3′	58°19′	58°10′	$h^1 \cdot a^1$	$100 \wedge 10\bar{1}$
$1 \wedge 8$	10	16.5′	43° 8′	43° 5′	$h^1 \cdot d^{1/2}$	$\bar{1}00 \wedge \bar{1}1\bar{1}$
$2 \wedge 11$	6	16.1′	33°26′	33°24′	$g^1 \cdot e^{1/2}$	$010 \wedge 02\bar{1}$
$1 \wedge 9$	5	—	41°47′	41°50′	$h^1 \cdot t$	$\bar{1}00 \wedge \bar{1}\bar{1}0$
$1' \wedge 7$	5	—	54°18′	54°26′	$h^1 \cdot b^{1/2}$	$100 \wedge 11\bar{1}$
$2' \wedge 10$	3	—	33°22′	33°40′	$g^1 \cdot i^1$	$0\bar{1}0 \wedge 0\bar{1}\bar{1}$
$1 \wedge 14$	2	—	25°29′	25°24′	$h^1 \cdot h^3$	$\bar{1}00 \wedge \bar{2}\bar{1}0$
$1' \wedge 12$	2	—	31°38′	31°53′	$h^1 \cdot {}_3a$	$100 \wedge 21\bar{1}$
$1' \wedge 13$	1	—	75°33′	74°56′	$h^1 \cdot b^1 d^{1/3} g^{1/2}$	$100 \wedge 12\bar{2}$

N.B.—The value of the *measured angle* is the *most probable value* given to the closest minute. The *probable error* is based on a value computed to the tenth of a minute; mention of the probable error has been omitted when the number of readings in the series is too small.

The Lévy form-symbols and the Miller face-symbols in the last two columns are in reference to the set of axial elements (VI).

A peculiar property of the crystals studied is the large number of well defined zones present: thirteen zones are found in each of which at least three forms occur. This fact simplifies the determination of the face symbols, *all of which* can be obtained from the

given five by applying only the "Addition and Subtraction Rule."[3] This can easily be seen from Fig. 1; the nine unknown symbols are found in the following order: **8', 5, 7, 9', 10', 12, 14', 11, 13.**

Simple trigonometric calculations lead to the axial elements:[4]

$$\breve{a}:\bar{b}:\dot{c} = 1.1082:1:1.0219,$$

$$\alpha = 105°14', \qquad \beta = 103°37', \qquad \gamma = 60°45', \qquad (I)$$
$$A = 79°58', \qquad B = 82°42', \qquad C = 117°4'.$$

The eleven angles which have been measured in addition to the five fundamental ones, are now computed from the latter. Their measured and computed values may be compared in Table 1.

IMPROVEMENT IN THE PRELIMINARY SET OF AXIAL ELEMENTS

When very many measurements are available, it is possible to find as many different unit-cells (or sets of axial elements) as there are ways of choosing five angles out of the number that are available. Provided all the measurements are about equally good, it is possible to combine them all in such a way as to obtain a *mean unit-cell* which is probably closer to the truth than any of the above. The method has been discussed by Mallard.[5] It leads to as many differential equations between the parameters of the polar lattice as there are superabundant measurements; the method of the least squares reduces them to five linear equations containing the corrections (to be applied to the parameters) as variables; these corrections being determined, it is easy to find the corrections to be made to the unit-cell. Friedel gives a somewhat modified method in his text-book.

We have attempted unsuccessfully to apply the method in the present case. The reason for its failure is that the preliminary unit-

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[3] Dr. Austin F. Rogers called attention to the value of this simple rule at the 1924 meeting of the *Mineralogical Society of America*, at Ithaca, N. Y., *Am. Min.*, **10**, 68, 1925; **11**, 303, 1926.

It may be interesting to know, in this connection, how the French crystallographer expresses this rule: "The plane *tangent to the edge* of two given faces (*hkl*) and (*pqr*) has the following indices:

$$h+p, \qquad\qquad k+q, \qquad\qquad l+r.$$

The plane *tangent to the supplementary edge* has the indices:

$$h-p, \qquad\qquad k-q \qquad\qquad l-r."$$

(See Friedel, *op. cit.*, p. 229).

[4] We use the abbreviated notation:

$$A = (010 \wedge 001), \quad B = (001 \wedge 100), \quad C = (100 \wedge 010),$$

for the sides of the spherical triangle 100.010.001.

[5] Traité de Cristallographie, Ernest Mallard, Tome I, p. 295, **1879.**

cell (I) had been determined from five measurements which were decidedly better than the others.

LAW OF HAÜY

Our unit-cell (I) satisfies the Law of Haüy, in its vaguest form, that is to say, that the face indices referred to this lattice are small integers.

Many other unit-cells can be found which fulfill the same condition. For instance, if we start from the same fundamental angles and the following symbols: $1'(001)$, $2(100)$, $4'(\bar{1}10)$, $3'(110)$, and $6'(\bar{1}01)$, we arrive at these results: $\breve{a}:\bar{b}:\dot{c}: = 0.9691:1:1.0196$,

$$\alpha = 105°14', \qquad \beta = 97°26', \qquad \gamma = 88°29', \qquad (II)$$
$$A = 74°50', \qquad B = 82°42', \qquad C = 90°28'.$$

This second unit-cell leads to simple indices; the indices are even simpler with cell (III), in which $\dot{c} = 0.5098$, all the other axial elements remaining as in (II). Cell (III) is found by starting from the same five fundamental angles and the symbols: $1'(001)$, $2(100)$, $4'(\bar{1}10)$, $3'(110)$, and $6'(\bar{2}01)$.

If $(h'k'l')$ is the symbol of a face referred to lattice (I), let $(h''k''l'')$ and $(h'''k'''l''')$ represent the same face referred to latices (II) and (III), respectively. The transformation formulae are:

$$h'' = 2h' - k', \qquad k'' = k', \qquad l'' = 2l',$$

and

$$h''' = 2h' - k', \qquad k''' = k', \qquad l''' = l'.$$

How are we to choose from all the possibilities?

LAW OF BRAVAIS

The answer to this question is: By applying the Law of Bravais.

We compute the reticular densities of the forms in the different cases, *i.e.* referred to the various lattices, and see in which one the list of forms arranged according to decreasing reticular densities is in best agreement with the *observed* order of importance.

The formula giving the area $S(hkl)$ of the elementary parallelogram (mesh or plane unit-cell) in the reticular plane (hkl) is known and may be written as follows for the triclinic system:

$S^2(hkl) = h^2S^2(100) + k^2S^2(010) + l^2S^2(001)$

$+2[hkS(100)S(010)\cos C + klS(010)S(001)\cos A + lhS(001)S(100)\cos B]$, in which

$$S(100) = bc \sin \alpha,$$
$$S(010) = ca \sin \beta,$$
$$S(001) = ab \sin \gamma.$$

Following Friedel, we compute the value S^2 instead of the reticular density, the latter being of course inversely proportional to S. The list of the first two hundred reticular planes is given in Table 2 in the order of decreasing densities for the first lattice (unit-cell I). Known forms, *i.e.* forms which occur on the crystals, are italicized.

TABLE 2

PLANES OF LATTICE (I) LISTED IN ORDER OF DECREASING RETICULAR DENSITIES OR INCREASING S^2.

No.	(I)	S^2	(I)	S^2	(I)	S^2	(I)	S^2
1	*001*	0.94	201	5.31	230	8.87	231	11.40
2	*100*	0.97	$12\bar{2}$	5.62	130	8.91	113	11.45
3	*110*	1.20	012	5.69	$30\bar{1}$	8.96	$32\bar{3}$	11.68
4	*010*	1.21	121	5.76	$21\bar{3}$	8.97	$42\bar{1}$	11.72
5	*$\overline{111}$*	1.52	112	6.16	311	9.03	$\bar{1}13$	11.97
6	*$\bar{1}01$*	1.66	021	6.52	$\bar{1}21$	9.23	$31\bar{3}$	12.12
7	*$0\bar{1}\bar{1}$*	1.78	$1\bar{1}2$	6.66	$12\bar{3}$	9.31	$43\bar{1}$	12.25
9	*101*	2.15	$31\bar{1}$	6.84	$23\bar{2}$	9.41	$41\bar{1}$	12.41
8	*011*	2.52	221	6.95	$22\bar{3}$	9.52	$03\bar{2}$	12.42
	111	2.74	310	7.00	122	9.55	$23\bar{3}$	12.49
10	*210*	3.12	$2\bar{1}0$	7.08	$33\bar{1}$	9.86	$\bar{1}22$	12.53
11	*$1\bar{1}0$*	3.17	$32\bar{1}$	7.14	$13\bar{2}$	9.94	410	12.82
	$21\bar{1}$	3.20	$\bar{1}12$	7.17	321	10.07	$3\bar{1}0$	12.92
	$11\bar{2}$	3.71	320	7.67	103	10.11	312	12.93
	$12\bar{1}$	3.79	$11\bar{3}$	7.77	301	10.41	031	12.95
	120	3.84	$\bar{1}20$	7.79	$1\bar{2}2$	10.54	$13\bar{3}$	13.26
	$1\bar{1}1$	3.98	$\bar{2}11$	7.90	$\bar{2}12$	10.59	$2\bar{2}1$	13.36
12	*$0\bar{1}2$*	4.21	$2\bar{1}1$	8.12	$03\bar{1}$	10.73	$\bar{3}11$	13.50
	$\bar{1}02$	4.23	$23\bar{1}$	8.20	013	10.74	331	13.54
	$\bar{1}11$	4.24	$1\bar{2}1$	8.23	$33\bar{2}$	10.83	$11\bar{4}$	13.70
	$20\bar{1}$	4.34	$12\bar{2}$	8.47	$\bar{2}03$	10.85	203	13.76
	$22\bar{1}$	4.49	$33\bar{1}$	8.49	$30\bar{2}$	11.04	$41\bar{2}$	13.88
	211	4.91	$0\bar{1}3$	8.51	$02\bar{3}$	11.04	$\bar{2}21$	13.88
13	*$0\bar{2}1$*	5.04	$31\bar{2}$	8.54	$2\bar{1}2$	11.04	302	13.94
	$21\bar{2}$	5.15	212	8.58	$1\bar{1}3$	11.20	213	14.11
14	*102*	5.20	$\bar{1}03$	8.66	131	11.20	$43\bar{2}$	14.18
	$3\bar{1}1$	14.22	$14\bar{1}$	16.60	114	18.61	$\bar{2}30$	20.72
	$24\bar{1}$	14.34	$\bar{1}31$	16.64	$\bar{1}14$	18.65	$1\bar{2}4$	20.76
	322	14.35	$14\bar{2}$	16.69	313	18.71	$\bar{3}04$	20.80
	430	14.61	$32\bar{4}$	16.76	$04\bar{1}$	18.84	$2\bar{3}1$	21.03
	$21\bar{4}$	14.66	$43\bar{3}$	16.78	$53\bar{1}$	19.00	$\bar{4}11$	21.05
	$0\bar{1}4$	14.69	$1\bar{3}2$	16.84	141	19.07	$40\bar{3}$	21.06
	$1\bar{2}3$	14.71	032	16.87	$52\bar{2}$	19.11	$43\bar{4}$	21.24
	$\bar{1}30$	14.84	223	16.88	412	19.24	133	21.39

TABLE 2 (Continued)

No.	(I)	S²	(I)	S²	(I)	S²	(I)	S²
	$12\bar{4}$	14.87	104	16.90	520	19.27	$0\bar{3}4$	21.41
	$1\bar{3}1$	14.90	$41\bar{3}$	17.21	$34\bar{1}$	19.43	214	21.51
	$\bar{1}04$	14.96	$3\bar{1}2$	17.38	$53\bar{2}$	19.49	$\bar{2}14$	21.58
	$34\bar{1}$	15.01	$23\bar{4}$	17.44	$3\bar{2}0$	19.52	041	21.80
	411	15.09	401	17.46	$14\bar{3}$	19.64	$52\bar{3}$	21.83
	421	15.14	$31\bar{4}$	17.57	$51\bar{1}$	19.93	$53\bar{3}$	21.84
	$\bar{2}13$	15.15	$1\bar{1}4$	17.62	$34\bar{2}$	20.07	$\bar{2}23$	21.87
	123	15.21	$44\bar{1}$	17.62	$44\bar{3}$	20.19	225	22.03
	132	15.36	431	17.62	$\bar{3}13$	20.27	233	22.07
	023	15.49	014	17.66	$\bar{1}32$	20.32	$51\bar{2}$	22.14
	$40\bar{1}$	15.52	$\bar{1}23$	17.71	$2\bar{2}3$	20.33	521	22.16
	$42\bar{3}$	15.78	$34\bar{3}$	18.07	530	20.39	$54\bar{1}$	22.18
	232	15.80	332	18.18	$32\bar{1}$	20.44	215	22.22
	$2\bar{1}3$	15.83	$52\bar{1}$	18.26	$\bar{3}21$	20.47	$4\bar{1}1$	22.25
	$\bar{3}12$	15.95	241	18.27	323	20.49	$\bar{2}31$	22.28
	340	16.28	$33\bar{4}$	18.37	510	20.58		
	140	16.41	$13\bar{4}$	18.45	$4\bar{1}0$	20.72		

N.B.—Symbols of known forms are italicized.

It is easy to see how well this list agrees with the observed facts (relative importance of the faces); there is only one exception: the order of faces **8** and **9** is reversed. The first nine forms in the list of decreasing reticular densities are all present. The tenth is unknown but the next two are present again. The other gaps are larger. The influence of disturbing factors, although very little known, probably becomes more important as we go down the list and may account for the vacant spaces. The importance of the last three forms, it must be admitted, is very small; they represent minor truncations, each of them has only been found once on the crystals examined.

The values of S^2 also show why faces **3** and **4, 1** and **2,** and (less plainly, it is true) **5** and **6** are about equally important.

We have computed the values of S^2 for many more forms than were necessary to check the agreement with the Law of Bravais. We have done this in order to show what small importance must be attached to the expression "simplicity of indices." It is instructive to read the list in that respect. Symbols containing 1, 2, and 3 as indices, for instance, range from $S^2 = 7.14$ (for $32\bar{1}$, 38th form) to $S^2 = 22.28$ (for $\bar{2}31$, 202nd form). Faces with "simple" indices

follow faces with higher indices, in a great many cases. No apparent law is to be inferred from the "simplicity" of the indices.

That the "simplicity" of the indices is not a sufficient reason to account for the presence or absence of a face, is shown even better by Table 3 where a series of forms with equally simple indices are

TABLE 3

LIST OF FORMS WITH EQUALLY SIMPLE INDICES REFERRED TO LATTICE (I)

Forms:	*001*	*100*	*010*									
S^2:	0.94	0.97	1.21									
	110	$\overline{1}01$	$0\overline{1}1$	*101*	*011*	$1\overline{1}0$						
	1.20	1.66	1.78	2.15	2.52	3.17						
	$\overline{11}1$	111	$1\overline{1}1$	$\overline{1}11$								
	1.52	2.74	3.98	4.24								
	210	120	$0\overline{1}2$	$\overline{1}02$	$20\overline{1}$	$0\overline{2}1$	*102*	201	012	021	$2\overline{1}0$	$\overline{1}20$
	3.12	3.84	4.21	4.23	4.34	5.04	5.20	5.31	5.69	6.52	7.08	7.79

N.B.—Known forms are italicized.

listed in the order of decreasing reticular densities. All the forms of the same series (same horizontal line), having similar indices, ought to have an equal opportunity to be present if the "simplicity of indices" were a sufficient criterion. We see, on the contrary, that all important known forms generally appear at the beginning of each series. The exception of the last three underlined forms has little weight in this discussion, for the reasons stated above. It is however significant that, although disturbing influences were unquestionably present, they cannot entirely counteract the dominant influence of the lattice, since the three forms that are exceptions still occur among the first seven of the twelve in the series.

Similar lists can be made for the second and third lattices (unit cells II and III). It immediately becomes obvious that these lattices do not express the facts observed with respect to the relative importance of existing forms. To give complete lists, such as that of Table 2, would increase the size of this paper beyond reasonable bounds. The important point is to know where the existing forms fall in the lists. We arranged the fourteen known forms in the order of decreasing reticular densities and for each one indicated the rank

TABLE 4

RANK OCCUPIED BY THE KNOWN FORMS IN THE LISTS OF FORMS ARRANGED ACCORDING TO DECREASING RETICULAR DENSITIES FOR LATTICES (I), (II), (III), (IV), (V) AND (VI)

	I				II				III				IV			V	VI
No.	Symbol	S²	Rank	No.	Symbol	S²	Rank	No.	Symbol	S²	Rank	No.	Symbol	S²	Rank	Symbol	Symbol
1	001	0.94	1	1	001	0.94	1	1	001	0.94	1	6	100	0.55	1	010	100
2	100	0.97	2	2	100	3.87	4	2	100	0.97	3	9	010	0.71	2	100	010
3	110	1.20	3	6	$\bar{1}01$	4.33	5	3	110	1.91	6	1	$1\bar{1}0$	1.25	3	001	001
4	010	1.21	4	9	101	5.29	6	4	$1\bar{1}0$	1.94	7	2	110	1.28	4	$\bar{1}01$	$0\bar{1}1$
5	$\bar{1}\bar{1}1$	1.52	5	3	110	7.65	11	5	$\bar{1}\bar{1}1$	2.11	8	4	001	1.60	6	$\bar{1}01$	$\bar{1}01$
6	$\bar{1}01$	1.66	6	4	$1\bar{1}0$	7.77	12	14	101	2.15	9	3	$\bar{1}11$	1.61	7	$0\bar{1}1$	$1\bar{1}0$
7	$0\bar{1}1$	1.78	7	13	$\bar{1}\bar{1}1$	8.20	13	7	$\bar{1}\bar{1}1$	2.63	11	5	$\bar{2}01$	2.12	9	$\bar{1}10$	$\bar{1}11$
9	101	2.15	8	5	$1\bar{1}2$	8.45	14	8	$\bar{1}11$	3.14	12	7	$\bar{1}11$	2.43	11	$\bar{1}11$	$1\bar{1}0$
8	011	2.52	9	14	102	8.59	15	6	$\bar{2}01$	4.33	18	8	$\bar{1}11$	3.27	17	$1\bar{1}0$	110
10	210	3.12	11	7	$\bar{1}12$	10.51	20	12	$1\bar{1}2$	5.19	26	11	$\bar{1}11$	4.15	23	$\bar{1}11$	$\bar{1}11$
11	$\bar{1}10$	3.17	12	8	$1\bar{1}2$	12.55	23	9	$\bar{2}01$	5.29	28	10	$\bar{2}21$	4.17	24	$\bar{1}01$	$0\bar{1}1$
12	$0\bar{1}2$	4.21	18	12	$1\bar{1}4$	20.75	47	13	$\bar{2}\bar{2}1$	8.20	45	12	$\bar{2}21$	5.75	37	$\bar{2}01$	$0\bar{2}1$
13	$0\bar{2}1$	5.04	24	10	$31\bar{0}$	38.50	99	10	$31\bar{0}$	9.62	58	13	$\bar{1}12$	6.82	49	$\bar{1}21$	$\bar{2}\bar{1}1$
14	102	5.20	26	11	$\bar{3}10$	38.87	103	11	$3\bar{1}0$	9.72	61	14	$\bar{1}30$	6.90	50	$\bar{2}12$	122
																120	210

N.B.—For Lattices (V) and (VI) the form number and rank are the same as for lattice (I). The value of S² in lattices (V) and (VI) is obtained by multiplying the S² of (I) by constant factors.

occupied in the complete list. Table 4 will permit comparison between the various lattices considered.

We observe that (except in lattice I) the order departs widely from the observed order of importance (1 to 14). Moreover, the known forms are among the first 26 in the first lattice, compared with the first 103, 61, and 50 in the other lattices. This shows how ill-adapted to the facts would be such unit-cells as (II) and (III).

<div align="center">PSEUDO-SYMMETRY</div>

It is often said to be advantageous to choose a particular set of axial elements in order to stress a certain pseudo-symmetry possessed by the crystal. This practice, however, is to be condemned when the unit-cell adopted to emphasize the pseudo-symmetry ignores the Law of Bravais.

Of this, the present study affords a striking example. It so happens that our crystals sometimes exhibit a pseudo-tetragonal symmetry, due to nearly equal development of the forms 1 and 2. Let us project the crystal on a plane perpendicular to the zone axis
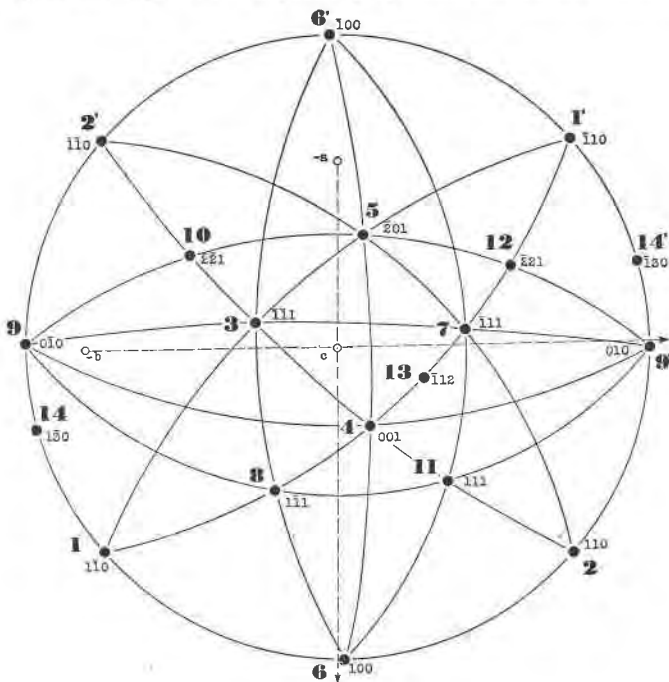
Fig. 2. Projection IV.

(1, 2). We see (Fig. 2) that the projection has a somewhat distorted tetragonal appearance, if we take the main faces only into account. It also shows the presence of a plane of pseudo-symmetry: the great circle **4, 5.** It must of course be observed that face **13** has no symmetrical equivalent on the left side of the projection (Fig. 2) and that neither **14** ($1\bar{3}0$) nor **14'** ($\bar{1}30$) is reflected in the plane of pseudo-symmetry. Nevertheless, the pseudo-symmetry is a fairly well marked feature. The question arises: Is it advisable to express this property by choosing a unit-cell *ad hoc?*

The following set of axial elements (see projection IV, Fig. 2) would answer that question:

$$\breve{a}:\bar{b}:\acute{c} = 1.2708:1:0.7580,$$
$$\alpha = 101°57', \quad \beta = 118°55', \quad \gamma = 85°13', \qquad \text{(IV)}$$
$$A = 78°59', \quad B = 61°26', \quad C = 88°53'.$$

This set of elements is derived from the same five fundamental angles as the other sets, by using the symbols **4**(001), **6**(100), **2**(110), **1'**($\bar{1}10$), and **3**($\bar{1}\bar{1}1$).

The transformation formulae from the first system to this one are:

$$h^{IV} = h' - l', \ k^{IV} = h' + l', \ l^{IV} = -k'.$$

The face symbols emphasize the pseudo-tetragonal symmetry as the forms **1** and **2,** on the one hand, and **6** and **9,** on the other, have the same indices. The presence of the plane of pseudo-symmetry is also brought out by the fact that **10** and **12, 3** and **7, 8** and **11** have similar symbols.

But when we list the forms in their order of decreasing reticular densities or increasing S^2 (Table 4), we realize that this new set (IV) of axial elements does not give a proper expression to the observed facts concerning the importance of faces. In the lattice defined by (IV) the Law of Bravais does not hold much better than in (II) or (III). Does this invalidate the law? No. It merely proves that the choice of the lattice is not proper. The Law of Bravais is independent of any theory, it is a law of observation which no new theory can disregard.

Are There Other Solutions?

If we turn the stereographic projection IV (Fig. 2) in its plane, and keep the same five fundamental angles but adopt the symbols **3**(001), **2'**(100), **1**(010), **6**($\bar{1}10$), and **4**($\bar{1}01$), we obtain a new projection and the following set of axial elements:

$$\breve{a}:\bar{b}:\acute{c} = 1.0473:1:0.9786,$$
$$\alpha = 105°14', \quad \beta = 115°22', \quad \gamma = 89°54', \qquad \text{(V)}$$
$$A = 73°9', \quad B = 63°40', \quad C = 82°42'.$$

If we list the forms of this lattice according to decreasing reticular densities and italicize the known forms, we get exactly the same results as in case (I) (see Table 4): all the known forms appear at the same places in the list, although with other symbols. The transformation formulae to pass from (I) to (V) are:

$$h^V = -h' + k', \; k^V = -l', \; l^V = -k'.$$

The values of S^2 in lattice (V) are exactly proportional to those of lattice (I). Denoting by $S(I)$ and $S(V)$ the reticular areas in lattices (I) and (V) respectively, we may write

$$S^2(V) = K \cdot S^2(I),$$

with $K = 0.917$.

Is this new solution (V) distinct from (I)? In other words does unit-cell (V) define the same lattice as unit-cell (I)? Or again, is the volume of unit-cell (I) equal to the volume of unit-cell (V)?

The formula giving the cell volume may be written as follows:
$$V = abc \; \sin\beta \; \sin\gamma \; \sin A = abc \; \sin\gamma \; \sin\alpha \; \sin B = abc \; \sin\alpha \; \sin\beta \; \sin C$$
for any given lattice. The unit of volume is the cube of the parameter b.

Before any two cell volumes can be compared, it must be determined that the unit in which the volumes are expressed is the same for both cells.

The Three Proportional Unit-Cells

It must be kept in mind that it is possible to express the volume of a given unit-cell in three different units, *viz*, the cubes of the three unit-lengths. The volume will be expressed by the smallest number when the largest unit-length is taken as $\bar{b}$, or in other words when, the unit-length of $\bar{b}$ being conventionally taken as unity, the unit-lengths of $\breve{a}$ and $'$ are both less than unity.

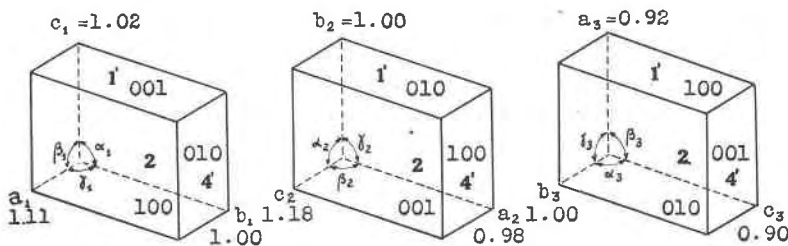As an example, let us consider (Fig. 3) the three axes of reference

FIG. 3. Cyclic permutations of the axial elements in the first octant. (N.B.—All three cells are purposely oriented in parallel positions so as to show the proportionality of the volumes.)

Oa, Ob, and Oc in our first lattice (I). The corresponding unit-lengths are

$$\breve{a}_1 : \bar{b}_1 : \acute{c}_1 = 1.1082 : 1 : 1.0219.$$

But we may choose any one of the three lengths as unit $\bar{b}$, if we change the names of the axes according to the proper cyclic permutation (leaving the system of reference right-handed). The above values, for instance, may be divided by 1.0219 and called $\acute{c}_2$, $\breve{a}_2$, $\bar{b}_2$ or divided by 1.1082 and designated $\bar{b}_3$, $\acute{c}_3$, $\breve{a}_3$, which leads to the two possibilities:

$$\breve{a}_2 : \bar{b}_2 : \acute{c}_2 = 0.9786 : 1 : 1.0845,$$
$$\breve{a}_3 : \bar{b}_3 : \acute{c}_3 = 0.9221 : 1 : 0.9023.$$

It is easy to see that the angles α, β, γ between the axes follow the same cyclic permutation, as do also the angles A ($010 \wedge 001$, B ($001 \wedge 100$), and C ($100 \wedge 010$).

Let

$$\alpha_1 = 105°14', \qquad \beta_1 = 103°37', \qquad \gamma_1 = 60°45',$$
$$A_1 = 79°58', \qquad B_1 = 82°42', \qquad C_1 = 117° \ 4'$$

be the values of these angles in the case of unit-cell (I), we have

$$\alpha_2 = \beta_1 \qquad \beta_2 = \gamma_1, \qquad \gamma_2 = \alpha_1,$$
$$A_2 = B_1, \qquad B_2 = C_1, \qquad C_2 = A_1;$$

and

$$\alpha_3 = \gamma_1, \qquad \beta_3 = \alpha_1, \qquad \gamma_3 = \beta_1,$$
$$A_3 = C_1 \qquad B_3 = A_1 \qquad C_3 = B_1.$$

From the above, it is clear that the volumes of the three cells will be in the ratio:

$$V' : V'' : V''' = a_1 b_1 c_1 : a_2 b_2 c_2 : a_3 b_3 c_3,$$

or, in the present instance,

$$V' : V'' : V''' = 1 : \left(\frac{1}{1.0219} \right)^3 : \left(\frac{1}{1.1082} \right)^3.$$

The three expressions of the cell volume in lattice (I) are:

$$V'(\text{I}) = 0.945, \quad V''(\text{I}) = 0.886, \quad V'''(\text{I}) = 0.694.$$

The same lattice is defined by any one of these three cells.

IDENTITY OF LATTICES (I) AND (V)

We find the following three expressions for the volume of cell (V):

$$V'(\text{V}) = 0.886, \quad V''(\text{V}) = 0.945, \quad V'''(\text{V}) = 0.771.$$

The volume of cell (I) and that of cell (V) are expressed by the same number 0.886 when the unit of length is the same in both cases, as can be easily ascertained.

It follows that the two unit-cells (I) and (V) define the same lattice (Fig. 4). It may happen that the Haüy-Bravais lattice is not definitely determined, that is to say one may, in certain cases,
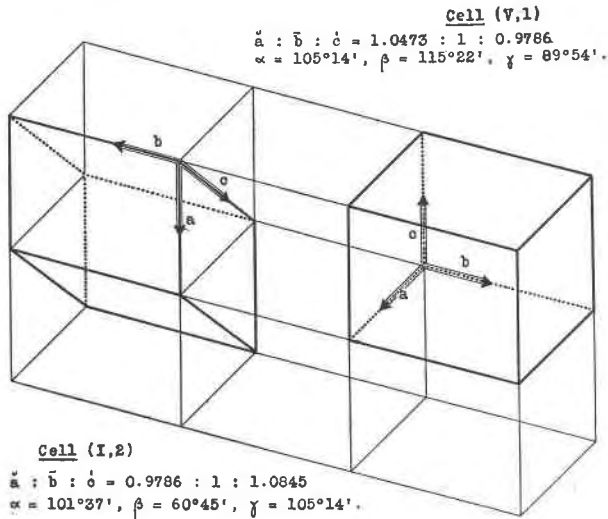

FIG. 4. Relationship between cells (I,2) and (V,1) which define the same lattice. (N.B.—The axial elements of cell (I, 2) are obtained from cell (I, 1) by the first cyclic permutation as explained above.)

hesitate between two or more lattices which comply equally well with the Law of Bravais. In this study we have not found any lattice, other than (I), to be in agreement with the Law of Bravais.

CHOICE OF THE UNIT CELL DEFINING THE HAÜY-BRAVAIS LATTICE

It may be interesting to observe that cell (V) brings out the remarkable value $\gamma = 89°54'$.

From the point of view of simplicity of indices, we see that the face symbols are simpler with cell (I) than with cell (V). In the former, all the known faces are found in the first four series, that is to say among 25 symbols containing either (0, 0, and 1), (0, 1, and 1), (1, 1, and 1), or (0, 1, and 2). With cell (V), the known faces occur among the 49 of six series, including the symbols formed with (1, 1, and 2), or (2, 2, and 1). (See Table 5.)

TABLE 5

SERIES OF EQUALLY SIMPLE FORM SYMBOLS LISTED ACCORDING TO DECREASING
DENSITIES IN SYSTEMS (I), (V), AND (VI)

(I)	*001*	*100*	*010*									
	110	$\overline{1}01$	$0\overline{1}1$	*101*	*011*	$1\overline{1}0$						
	$\overline{1}11$	111	$1\overline{1}1$	$\overline{1}11$								
	210	*120*	$0\overline{1}2$	$\overline{1}02$	$\overline{2}01$	$0\overline{2}1$	*102*	201	012	021	$2\overline{1}0$	$\overline{1}20$
(V)	*010*	*100*	*001*									
	$10\overline{1}$	$1\overline{1}0$	$1\overline{1}0$	*110*	011	*101*						
	$\overline{1}11$	$\overline{1}11$	$11\overline{1}$	111								
	$\overline{2}01$	$0\overline{2}1$	$\overline{1}02$	$1\overline{2}0$	$\overline{2}10$	$0\overline{1}2$	*120*	210	021	012	201	102
	$\overline{1}12$	$\overline{2}11$	$\overline{1}2\overline{1}$	$\overline{2}11$	$1\overline{2}1$	$\overline{1}21$	$1\overline{1}2$	$\overline{1}12$	$2\overline{1}1$	121	211	112
	$\overline{2}12$	$\overline{1}22$	$\overline{2}12$	$2\overline{2}1$	$\overline{2}21$	$1\overline{2}2$	$2\overline{2}1$	$\overline{1}22$	$2\overline{1}2$	221	122	212
(VI)	*100*	*010*	*001*									
	$0\overline{1}1$	$\overline{1}01$	$1\overline{1}0$	*110*	101	*011*						
	$\overline{1}11$	$1\overline{1}1$	$\overline{1}11$	111								
	$0\overline{2}1$	$\overline{2}01$	$0\overline{1}2$	$2\overline{1}0$	$\overline{1}20$	$\overline{1}02$	*210*	120	201	102	021	012
	$\overline{1}\overline{1}2$	$\overline{1}21$	$\overline{2}1\overline{1}$	$1\overline{2}1$	$\overline{2}11$	$2\overline{1}1$	$\overline{1}12$	$1\overline{1}2$	$\overline{1}21$	211	121	112
	$\overline{1}22$	$\overline{2}\overline{1}2$	$1\overline{2}2$	$2\overline{2}1$	$2\overline{2}1$	$\overline{2}12$	$\overline{2}21$	$2\overline{1}2$	$\overline{1}22$	221	212	122

N.B.—Known forms are italicized.

But there are innumerable unit-cells, with different shapes, defining the same lattice, such as unit-cells (I) and (V) in the present instance. Which one should be adopted? There is no definite rule relative to this matter, except in certain cases of pseudo-symmetry.[6]

We adopt the unit-cell which has the smallest primitive translations (or parameters $\breve{a}$, $\bar{b}$, $\dot{c}$). One must be careful to measure the translations to be compared in terms of the same unit of length (Fig. 4). An easy rule to follow to see whether a given unit-cell should not be replaced by some other having shorter primitive

[6] In the case of *epidote*, for instance, G. Friedel shows that the usually adopted axial elements:

$$\breve{a}:\bar{b}:\dot{c}=1.5787:1:1.8036, \quad \beta=64°37',$$

although correctly defining the Haüy-Bravais lattice are poorly chosen because they do not bring out the remarkable pseudo orthorhombic symmetry.

He suggests to refer epidote to the following system of axes: new a-axis = old [$\overline{1}00$], new b-axis = old [010], new c-axis = old [102] and to center face (010). The new axial elements:

$$\breve{a}:\bar{b}:\dot{c}=1.5787:1:3.2590, \quad \beta=89°26',$$

stress the pseudo-symmetry ($\beta=89°26'$) as the faces which have nearly equal reticular densities are denoted by similar face symbols. (G. Friedel, *op. cit.*, p. 140.)

translations is to calculate the lengths of the face-diagonals and body-diagonals of the first cell. If any diagonal is found that is shorter than one selected for the primitive translations, then this diagonal should be taken as a parameter and substituted for the largest of the original translations.

Let us compute the diagonals of cell (I, 2) in which the unit length $\bar{b}$ is the same as in cell (V, 1). Graphically, by obliquely projecting all the lattice points of (I) onto a plane of the cell (I, 2), the projecting lines being parallel to the zone axis defined by the other two cell faces, it can be determined whether a face diagonal is shorter than any of the original translations. In case of doubt, or for accurate determination, the distance formula is used. The latter can be written as follows:

$$d^2 = u^2a^2 + v^2b^2 + w^2c^2 + 2\ uv \cdot ab \cdot \cos\gamma + 2\ vw \cdot bc \cdot \cos\alpha + 2\ wu \cdot ca \cdot \cos\beta,$$

where d is the parameter of a lattice row $[uvw]$, and the row indices u, v, w are supposed to be cleared of common factors.

We reach the conclusion that one diagonal of cell (I, 2) is shorter than one of the cell translations. The face diagonal of face 1, whose symbol is (010), when referred to (I, 2), is found to be equal to 1.0473. The new cell should then be constructed on this diagonal (1.0473) and the two smallest original translations, 0.9786 and 1. It is found to be identical with cell (V).

Cell (V) is, therefore, chosen to define the Haüy-Bravais lattice in preference to (I).

The Eight Octants in a Triclinic System of Reference and the 24 Possible Expressions of the Same Unit Cell

The three triclinic axes of reference are the intersections of the three co-ordinate planes in a Cartesian system of oblique co-ordinates. Three such planes divide space into eight octants. The first octant is defined as that formed by the positive directions of the three axes. We may take any of the eight octants for our first octant if we give proper signs to the axes.

The eight possibilities may be visualized by considering (Fig. 5) the primitive parallelopiped (V). The origin of the co-ordinates may be taken at any one of the eight corners, the three edges intersecting at that corner being taken as axes. Moreover, at each corner, there are three possible cyclic permutations (leaving the system of reference right handed), hence a total of 24 possible ways of expressing the axial elements of the same unit cell.
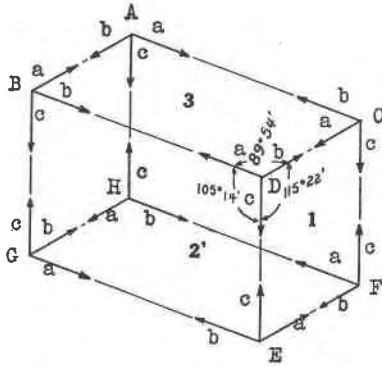
FIG. 5. The eight octants in a triclinic system of reference.

How to Limit the Choice

The axis of the main zone will be placed vertically. This axis is represented by the intersection of the two most important forms: in the present case, **1** and **2**. This condition reduces the number of possible expressions to eight. The origin of the co-ordinates being taken at any corner of the cell (A, B, C, D, E, F, G, or H), the choice of one axis (here the $\breve{c}$-axis) uniquely defines the system of reference, which must be right handed.

If it is desired to have the $\breve{a}$-axis sloping down toward the observer, then the angle β must be greater than 90°. Among the four different values which β may assume in the eight reference systems now being considered, two are greater than 90° (105°14′ and 115°22′), the other two are their supplements. This new condition reduces the number of possible expressions to four (corners B, D, G, or H).

Now if the unit lengths $\breve{a}$ and $\bar{b}$ are so chosen that $\breve{a}$ is the shorter (as in the orthorhombic system), we are left with only two possible sets of axes (G and D) out of the four. Their interaxial angles are:

$$\alpha = 64°38', \qquad \beta = 105°14', \qquad \gamma = 90°\ 6',$$

and

$$\alpha = 115°22', \qquad \beta = 105°14', \qquad \gamma = 89°54'.$$

The latter set (corner D) is selected in order that the stereographic projection of the basal pinacoid may fall in the lower right quadrant of the primitive circle.

FINAL SET OF AXIAL ELEMENTS

The parameters are proportional to those of cell (V) divided by 1.0473.

$$\breve{a}:\bar{b}:\mathring{c}=0.9548:1:0.9344,$$

$$\alpha=115°22', \qquad \beta=105°14', \qquad \gamma=89°54', \qquad \text{(VI)}$$

$$A=\ 63°40', \qquad B=\ 73°\ 9', \qquad C=82°42'.$$

The transformation formulae

$$h^{\text{VI}}=-l',\ k^{\text{VI}}=k'-h',\ l^{\text{VI}}=-k',$$

give the symbol $(h^{\text{VI}}k^{\text{VI}}l^{\text{VI}})$ of a face in system (VI) when its indices $(h'k'l')$ are known in system (I).

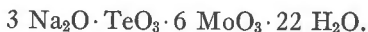The new orientation is seen in the stereographic projection (VI), (Fig. 6).
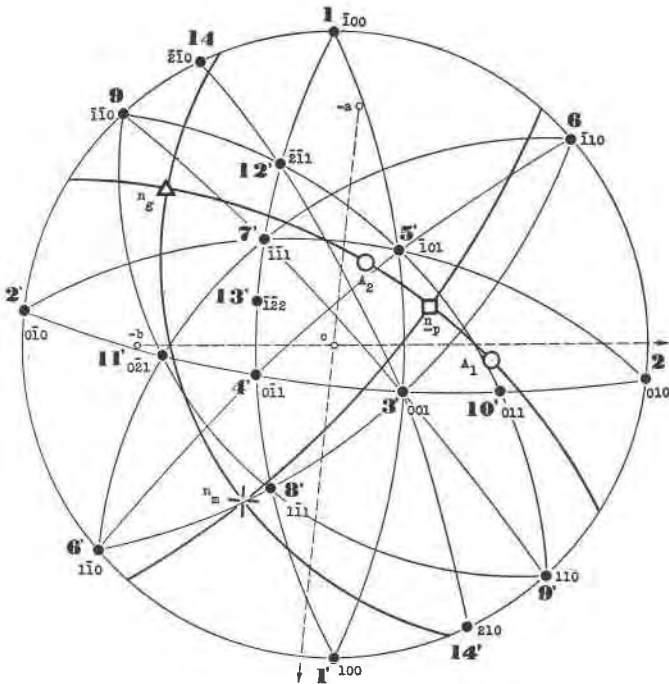
FIG. 6. Projection VI.

PART II. CRYSTALLOGRAPHIC DATA FOR SODIUM
MOLYBDO-TELLURATE

GENERAL. This new compound has the following *chemical formula*, according to Professor S. R. Wood who prepared it:

$$3 Na_2O \cdot TeO_3 \cdot 6 MoO_3 \cdot 22 H_2O.$$

Its *specific gravity* is 2.58 ± 0.02. Due to the solubility of the substance in water, the specific gravity was determined in ether and corrected for water.

The *hardness* is $2\frac{1}{2}$.

Sodium molybdo-tellurate crystallizes readily from a water solution forming perfectly developed small crystals, ranging in size from one millimeter or less to about five millimeters in cross section. The faces of a crystal will whiten and lose their reflecting power if left too long in dry, warm air.

FORM. The crystals belong to the pinacoidal or holohedral class of the triclinic system (Fig. 7).

The axial elements are:

$$\breve{a}:\bar{b}:\acute{c} = 0.9548:1:0.9344,$$

$\alpha = 115°22'$,	$\beta = 105°14'$,	$\gamma = 89°54'$,
$A = 63°40'$,	$B = 73°9'$,	$C = 82°42'$.

Fourteen forms have been observed. They are in order of their importance: $h^1\{100\}$ and $g^1\{010\}$, $p\{001\}$ and $e^1\{0\bar{1}1\}$, $a^1\{\bar{1}01\}$ and $m\{1\bar{1}0\}$, $b^{1/2}\{\bar{1}11\}$ and $d^{1/2}\{1\bar{1}1\}$, $t\{110\}$, $i^1\{011\}$, $e^{1/2}\{0\bar{2}1\}$, $\{\bar{2}11\}$, $\{\bar{1}22\}$, $\{210\}$. The last three forms are very rare.

The faces are numbered in order of their importance on the stereographic projection (Fig. 6). The list of faces according to decreasing reticular densities can be found in Table 4 (last column).

Interfacial angles: the list of measured and computed angles is given in Table 1.

HABIT. Usually tabular parallel to either $h^1\{100\}$ or $g^1\{010\}$, the crystals also, though more rarely, exhibit a short prismatic habit together with a pseudo-tetragonal appearance due to equal development of $h^1\{100\}$ and $g^1\{010\}$. The main zone, or zone of elongation, is almost invariably [001] defined by the same two forms. Probably all the faces of this zone are striated; the striations, however, are most distinctly visible on $h^1\{100\}$ and $g^1\{010\}$, usually better on the former than on the latter, and also on $p\{001\}$.
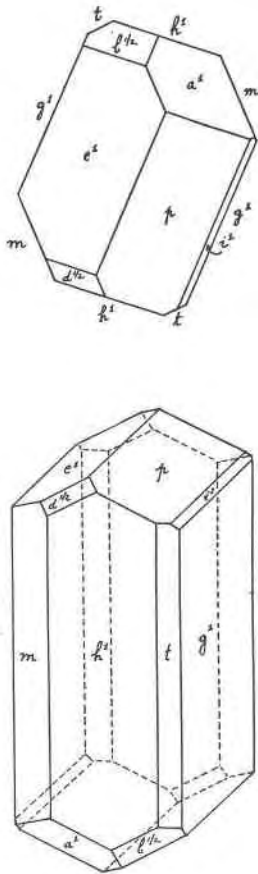
Fig. 7. A typical crystal of sodium molybdo-tellurate showing the ten principal forms, the usual prismatic habit, and a tendency towards pseudo tetragonal symmetry. (Horizontal plan and clinographic projection in the standard position: 18°30′ rotation and 9°30′ tilt. Drawn from the stereographic projection VI, Fig. 6.)

The crystals usually show a number of modifications. Some faces may be slightly hopper-shaped. This has often been observed for the face on which the growing crystal lies at the bottom of the crystallizing vessel.

CLEAVAGE, GLIDING, TWINNING. None of these discontinuous vectorial properties could be detected.

OPTICAL DATA. The sodium molybdo-tellurate crystals are colorless to whitish, transparent to translucent, with vitreous luster.

The crystals are biaxial and negative. $n_p = 1.577$, $n_m = 1.662$, $n_g = 1.683$; all three indices ± 0.003. $2V = 50\frac{3}{4}° \pm \frac{3}{4}°$.

The optical orientation is as follows:

Angle	$h^1(100)$	$g^1(010)$	$p\ (001)$	Φ	Λ
n_p	$102\frac{1}{2}°$	$58\frac{1}{2}°$	$29\frac{1}{2}°$	$331\frac{1}{2}°$	$36\frac{1}{2}°$
n_m	$42°$	$110°$	$63°$	$114\frac{1}{2}°$	$59\frac{1}{2}°$
n_g	$129°$	$140°$	$102\frac{1}{2}°$	$216°$	$72\frac{1}{2}°$
A_1	$85\frac{1}{2}°$	$36°$	$30°$	$359°$	$54°$
A_2	$119\frac{1}{2}°$	$82°$	$47°$	$285°$	$32\frac{1}{2}°$

The first meridian is passed through the pole (010). Longitudes represented by Φ are measured clockwise. The Λ values designate colatitudes.

The extinction angle, measured against the edge between $h^1(100)$ and $g^1(010)$, is

$$\text{on } h^1(100) = 34°, \qquad \text{on } g^1(010) = 17°.$$

The optical orientation is plotted on projection VI (Fig. 6).

Dispersion: $\rho > v$. The dispersion is greater for one axis than for the other.

OPTICAL MEASUREMENTS. A fair biaxial figure can usually be obtained in convergent light, simply by examining a few crushed fragments.

The refractive indices were determined partly by the ordinary immersion method, partly by calculation, as follows:

(1) By immersion. We found that n_p had a value between 1.560 and 1.591. The relief is high in monobrombenzol (1.560) and very low in trihydrobromine (1.591); n_m is slightly above 1.650 (α-monobromnaphthalene); n_g is intermediate between 1.650 and 1.74 (methylene iodide), with a higher relief in the latter than in the former.

(2) By measurement of double refraction. The difference between $n_g - n_m$ was measured four times by means of a Berek compensator, with an average value of 0.021.

(3) By measurement of 2V. The axial angle was measured on the Fedorov universal stage.

(4) By calculation. The size of 2V was computed for several sets of values assigned to the indices within permissible limits, in agreement with the above listed observations. For a given n_p, there is

only one value of n_m which leads to $2V = 50\frac{3}{4}°$ (as $n_g = n_m + 0.021$). The curve of n_m plotted against n_p provides two values (n_m, n_p) when 2V is kept constant and equal to $50\frac{3}{4}°$. We now make use of the observation that n_p shows the same amount of relief in 1.591 as n_m in 1.650. The point on the curve which is equally distant from $n_p = 1.591$ and $n_m = 1.650$ is easily located. Its coordinates are the values adopted for n_p and n_m.

The formula, $\tan V = \dfrac{n_p}{n_0} \sqrt{\dfrac{n_g{}^2 - n_m{}^2}{n_m{}^2 - n_p{}^2}}$ leads to $2V = 50°40'$ for the adopted set of indices.

The optical orientation was determined by measuring the angles which the directions of the principal refractive indices and optic axes make with the three unit faces. The measurements obtained on the universal stage are listed in the first three columns of the table. The longitudes and colatitudes were measured on a large scale stereographic projection.

The two extinction angles given above (34° and 17°), measured with the microscope, check the values read from the stereographic projection ($33\frac{1}{2}°$ and 16° respectively).